

phenoxide anion

Inchi: InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H/p-1
InchiKey: ISWSIDIOOBJBQZ-UHFFFAOYSA-M
Formula: C6H5O-
SMILES: [O-]c1ccccc1
Mol. weight [g/mol]: 93.10
CAS: 3229-70-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	0.760		Crippen Method
mcvol	75.360	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3229707&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/13-197-9/phenoxide-anion.pdf>

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